Strong coupling analysis of QED_3 for excitation spectrum broadening in undoped high-temperature superconductors

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Theory of quantum electrodynamics in three spatial-time dimension is applied to the two-dimensional $S = 1/2$ quantum Heisenberg antiferromagnet in order to investigate a doped hole in high-temperature superconductors. Strong coupling analysis of the U(1) gauge field interaction is carried out to describe spectral broadening observed in the undoped compounds. It is found that the fermionic quasiparticle spectrum is of Gaussian form with the width about $3J$, with J being the superexchange interaction energy. The energy shift of the spectrum is on the order of the quasiparticle band width, which suggests that the system is in the strong coupling regime with respect to the gauge field interaction describing the phase fluctuations about the staggered flux state.

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I. INTRODUCTION

One of the most fundamental questions about high-temperature superconductivity is how to describe doped holes introduced in the CuO_2 plane. The simplest way to approach this problem is to investigate the single hole doped system. Experimentally, the excitation spectrum associated with a single hole is observed by angle resolved photoemission spectroscopy (ARPES) in the undoped compounds such as $Sr_2CuO_2Cl_2$[1,2] and $Ca_2CuO_2Cl_2$.[3] Although the spectrum is not sharp but quite broad, whose width is ranging from 0.1eV to 0.5eV, the experiments show that the trace of the peak indicates a dispersion whose maxima are at $(\pm\pi/2, \pm\pi/2)$. The dispersion near these points is quadratic and almost isotropic. The band width is $2.2J \simeq 270$meV with J the superexchange interaction. This band width is much smaller than the band-structure estimation of $8t \simeq 2.8$eV. Furthermore, the observed spectra are not described by a conventional Lorentzian form but described by a Gaussian form.[4] These observations suggest that the quasiparticle excitations in the undoped cuprates are quite different from conventional Fermi liquid quasiparticles.

In the slave-fermion theory of the t-J model, the single hole system has been analyzed by the self-consistent Born approximation.[5] The effect of the spin-wave excitations is included in the self-energy in a self-consistent manner with omitting vertex corrections. The resulting hole dispersion has minima at $(\pm\pi/2, \pm\pi/2)$, and the band width is scaled by J. The dispersion along $(0, 0)$ to (π, π) is in good agreement with the experiments. Quantum Monte Carlo simulations based on a model, in which canonically transformed spinless fermions propagate with antiferromagnetic spin correlation background, like the slave-fermion formalism, are consistent with this result.[6] However, the dispersion along $(\pi, 0)$ to $(0, \pi)$ is much smaller than that in the experiments. This discrepancy is improved by including the next nearest neighbor and the third nearest neighbor hopping terms.[7] This suggests that within this approach the quadratic behavior near the $(\pi/2, \pi/2)$ point along $(0, \pi)$ to $(\pi, 0)$ has a different origin from that along $(0, 0)$ to (π, π). Furthermore, it turns out that the damping effect due to the coupling with the spin-wave modes does not lead to a broad line shape.[8] Recently Mischenko and Nagaosa studied a coupling to an optical phonon.[9] They numerically summed over Feynman diagrams including vertex corrections for phonons. It was argued that the coupling is in the strong coupling regime, and so the quasiparticle spectrum becomes broad. In this scenario the most enigmatic feature of the hole spectral broadening in the undoped compounds is associated with phonon effects. The dominant role is not played by the antiferromagnetic correlations which is believed to be essential for the mechanism of high-temperature superconductivity.

Here I take a different approach. I consider the staggered flux state proposed in the literature[10,11] from a mean field theory of the $S = 1/2$ antiferromagnetic Heisenberg model based on a fermionic representation of the spins. The dispersion of the quasiparticle in the staggered flux phase is in good agreement with the experimentally obtained dispersion as pointed out by Laughlin.[12] Including phase fluctuations about the mean field, the effective theory is described by quantum electrodynamics in three spatial-time dimension, which is called QED_3. At mean field level, the fermions are massless. By including the effect of the gauge field, the mass of the Dirac fermions is induced.[13] This mass is associated with the staggered magnetization. The presence of the mass term is also suggested by a variational Monte Carlo approach.[14] The quadratic dispersion around $(\pi/2, \pi/2)$ observed in the experiments is consistent with the massive quasiparticle spectrum. Furthermore, the quasiparticle dispersion is isotropic at $(\pi/2, \pi/2)$.

The purpose of this paper is to argue that the coupling of the fermions with the phase fluctuations leads to a broad Gaussian spectrum. The QED_3 action with the mass term is analyzed by performing a canonical transformation. The spectral function is obtained by calculating the Green's function of the Dirac fermion which is associated with a

single quasiparticle propagation. It is shown that the spectral function shows a broad Gaussian peak whose width is on the order of J.

The rest of the paper is organized as follows. In Sec.II, we describe the QED_3 formalism of the staggered flux state. After taking the transverse gauge, a canonical transformation is applied. The quasiparticle Green's function is computed in Sec.III. The spectral function is obtained with including vertex functions arising from random phase approximation about the instantaneous longitudinal gauge field interaction. Implications of the result is discussed in IV.

II. QED$_3$ THEORY OF THE STAGGERED FLUX STATE

For the description of the $S = 1/2$ two-dimensional quantum Heisenberg antiferromagnet, I take the following QED_3 action in the real time formalism as the effective theory:

$$S = \int d^3x \left[\overline{\psi}(x) \left[i\gamma^\mu \left(\partial_\mu - i a_\mu \right) - m\sigma_3 \right] \psi(x) - \frac{1}{4e_a^2} f_{\mu\nu} f^{\mu\nu} \right], \tag{2.1}$$

where the Dirac fermion fields, $\psi(x)$, consist of four component associated with even and odd sites and two independent nodes. Due to the spin degrees of freedom there are two species of $\psi(x)$. (For the derivation, see Appendix A.) Hereafter the spin index for $\psi(x)$ is suppressed because the spin degrees of freedom does not play an important role in the following calculation. The action (2.1) describes low-lying excitations around $(\pm\pi/2, \pm\pi/2)$ because the above continuum model was derived by taking the continuum limit at those points. Note that the theory is particle-hole symmetric. Therefore, the quasiparticle properties are identical to the quasihole properties.

For the gauge, I take the transverse gauge: $\nabla \cdot \mathbf{a} = 0$. In this gauge, the interaction between the fermions mediated by the longitudinal part of the gauge field is instantaneous as in the conventional electromagnetic field formulation:

$$\begin{aligned} S &= \int d^3x \overline{\psi}(x) \left[i\gamma^0 \partial_t + i\gamma^j \left(\partial_j + i a_j \right) - m\sigma_3 \right] \psi(x) \\ &+ \frac{e_a^2}{4\pi} \int d^3x \int d^2\mathbf{r}' \left[\rho(\mathbf{r}, t) - \rho_0 \right] \left[\rho(\mathbf{r}', t) - \rho_0 \right] \ln |\mathbf{r} - \mathbf{r}'| \\ &+ \frac{1}{2e_a^2} \int d^3x \left[\left(\partial_t \mathbf{a} \right)^2 - \left(\nabla \times \mathbf{a} \right)^2 \right], \end{aligned} \tag{2.2}$$

where the background gauge charge, $-e_a\rho_0$, comes from the constraint on the fermion number to represent the spin 1/2. In three spatial-time dimension, the "Coulomb" interaction is described by $V(r) = -\frac{e_a^2}{2\pi} \ln r$. Under the transverse gauge, the vector potential is represented by

$$a_x(q) = -\frac{iq_y}{q} a(q), \qquad a_y(q) = \frac{iq_x}{q} a(q), \tag{2.3}$$

in the momentum space. Quantizing the transverse gauge field, the Hamiltonian is

$$\begin{aligned} H &= \int d^2\mathbf{r} \overline{\psi}(\mathbf{r}) \left(-i\gamma^j \partial_j + m\sigma_3 \right) \psi(\mathbf{r}) + \int d^2\mathbf{r} \sum_q e^{iq\cdot\mathbf{r}} \overline{\psi}(\mathbf{r}) \frac{i}{q} \left(q_x \gamma_y - \gamma_x q_y \right) \sqrt{\frac{e_a^2}{2\omega_q}} \left(b_q + b_{-q}^\dagger \right) \psi(\mathbf{r}) \\ &+ \frac{1}{2} \int d^2\mathbf{r} \int d^2\mathbf{r}' V(|\mathbf{r} - \mathbf{r}'|) \left[\rho(\mathbf{r}) - \rho_0 \right] \left[\rho(\mathbf{r}') - \rho_0 \right] \\ &+ \sum_q \frac{\omega_q}{2} \left(b_q b_q^\dagger + b_q^\dagger b_q \right). \end{aligned} \tag{2.4}$$

In order to investigate the strong coupling effects, I perform the following canonical transformation[15]:

$$\overline{H} = e^s H e^{-s}, \tag{2.5}$$

where

$$s = \int d^2\mathbf{r} \sum_q \left(b_q - b_{-q}^\dagger \right) \psi^\dagger(\mathbf{r}) M_q(\mathbf{r}) \psi(\mathbf{r}). \tag{2.6}$$

(The area of the system is set to unity.) This is a unitary transformation if $M^{\dagger}_{-q}(\mathbf{r}) = M_q(\mathbf{r})$. The function $M_q(\mathbf{r})$ is chosen so that the interaction term between the Dirac fermions and the gauge field is cancelled by $[s, H]$:

$$M_q(\mathbf{r}) = -\sqrt{\frac{e_a^2}{2\omega_q^3}} e^{iq\cdot\mathbf{r}} \frac{i}{q} \gamma_0 \left(q_x\gamma_y - \gamma_x q_y\right). \tag{2.7}$$

Under this canonical transformation, the fermion fields transform as

$$e^s \psi(\mathbf{r}) e^{-s} = e^{X(\mathbf{r})} \psi(\mathbf{r}). \tag{2.8}$$

The function $X(\mathbf{r})$ is,

$$X(\mathbf{r}) = -\sum_q \left(b_q - b^{\dagger}_{-q}\right) M_q(\mathbf{r}). \tag{2.9}$$

III. QUASIPARTICLE GREEN'S FUNCTION

Now I compute the time-ordered Green's function:

$$\begin{aligned} G(\mathbf{r}, t) &= -i\left\langle T\psi(\mathbf{r}, t)\psi^{\dagger}(0,0)\right\rangle \\ &= -i\left\langle T\mathrm{e}^{X(\mathbf{r},t)}\psi(\mathbf{r}, t)\psi^{\dagger}(0,0)\mathrm{e}^{-X(\mathbf{0},0)}\right\rangle_{\overline{H}}. \end{aligned} \tag{3.1}$$

This Green's function has a matrix form of 4×4. But the matrix is divided into two blocks in which each part describes either the Dirac fermion fields near $(\pi/2, \pi/2)$ or the Dirac fermion fields near $(-\pi/2, \pi/2)$. It is enough to focus on one of them because two components are decoupled as far as long-wave length gauge field fluctuations are concerned. The superscript (1) is used to denote the former. Diagonalizing the factor with γ matrices, $X(\mathbf{r})$ is

$$X^{(1)}(\mathbf{r}) = i\sum_q \left(b_q e^{iq\cdot\mathbf{r}} + b_q^{\dagger} e^{-iq\cdot\mathbf{r}}\right)\sqrt{\frac{e_a^2}{2\omega_q^3}} U_q \tau_3 U_q^{\dagger}, \tag{3.2}$$

where

$$U_q = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -(q_x - iq_y)/q \\ (q_x + iq_y)/q & 1 \end{pmatrix}. \tag{3.3}$$

The first term in Eq.(2.4), which does not change its form by the canonical transformation, is diagonalized by a unitary transformation as well. Finally, by making use of the following formula,

$$\left\langle e^{Ab^{\dagger}+Bb} e^{Cb^{\dagger}+Db}\right\rangle = e^{\frac{1}{2}(AB+CD+2BC)} e^{(A+C)(B+D)n(\omega)}, \tag{3.4}$$

for bosons, Eq.(3.1) is

$$G^{(1)}(\mathbf{r}, t) = -i\sum_k e^{i\mathbf{k}\cdot\mathbf{r}} e^{-iE_k t} R_k \exp\left[-K(\mathbf{r}, t)\right], \tag{3.5}$$

at $T = 0$. The retarded Green's function has the same form for $t > 0$. Here,

$$R_k = \prod_{\mathbf{q}} \left[\frac{1}{4}\left(1 + \frac{k_x q_y - k_y q_x}{q\sqrt{k^2 + m^2}}\right)\right], \tag{3.6}$$

$$K(\mathbf{r}, t) = \sum_q \frac{e_a^2}{2\omega_q^3}\left(1 - e^{-i\omega_q t} e^{i\mathbf{q}\cdot\mathbf{r}}\right). \tag{3.7}$$

Performing the Fourier transform, the spectral function $A^{(1)}(\mathbf{k}, \omega)$ is given by $A^{(1)}(\mathbf{k}, \omega) = -\frac{1}{\pi}\mathrm{Im}G^{(1)}(\mathbf{k}, \omega)$.

So far the bare vertex function has been used for the computation. However, in the long-wave length limit taking the bare vertex is not appropriate as manifestly seen by infrared divergence in $K(\mathbf{r}, t)$. For the vertex part, random

phase approximation is applied with respect to the longitudinal interaction term. The bare vertex is reduced by the factor of $1/(1-\pi_q)$, where

$$\pi_q = v_q \sum_k Tr\left[G_k \gamma_0 G_{k+q} \gamma_0\right] = -\frac{m e_a^2}{\pi}\frac{1}{q^2} + O(1), \tag{3.8}$$

with $v_q = e_a^2/q^2$. For this computation, it is convenient to use the Euclidean formalism because the main contribution comes from π_q with $q = (\mathbf{q}, 0)$, where the Minkowskiian formalism leads to the same result.

Including the vertex correction the function $K(\mathbf{r}, t)$ is,

$$K(\mathbf{r}, t) = \frac{e_a^2}{2}\int_0^{\Lambda} dq \frac{1}{q^2}\left(\frac{1}{1-\pi_q}\right)^2 \left[1 - \mathrm{e}^{-i\omega_q t} J_0(qr)\right], \tag{3.9}$$

with $J_0(x)$ the zero-th order of the Bessel function of the first kind. The ultraviolet cutoff Λ introduced here because the wave length of fluctuations is larger than the lattice constant. The integrand is expanded with respect to q, before the integration. The result is

$$K(\mathbf{r}, t) \simeq i E_s t + \frac{1}{8}\Delta^2 r^2 + \frac{1}{4}\Delta^2 t^2, \tag{3.10}$$

where

$$E_s = \frac{e_a^2}{4}\log\left(\frac{\pi \Lambda^2}{e m e_a^2}\right), \tag{3.11}$$

$$\Delta^2 = \frac{e_a^2 \Lambda}{2\pi}. \tag{3.12}$$

The first term in Eq.(3.9) represents the energy shift, E_s. The shape is changed to a broad Gaussian form by the subsequent terms as shown below. For the factor R_k, the analytic expression was not obtained. From a numerical computation I found that R_k is linear in k at $0 < k < k_c$, with $k_c \simeq 1$, and reaches a saturated value of 0.2 for $k > k_0$. To approximate R_k, I took an approximate form of $R_k \simeq 0.2k$. In computing the Fourier transform, it is useful to note that the integration with respect to $\mathbf{r}$ and that with respect to t are carried out separately. For $k \ll \Delta$, I obtained

$$A^{(1)}(\mathbf{k}, \omega) \simeq \frac{0.10}{\sqrt{8\pi^2}} \exp\left[-\frac{(\omega - E_k - E_s)^2}{\Delta^2}\right]. \tag{3.13}$$

Therefore, the Dirac fermion energy spectrum is shifted by E_s and is a Gaussian form with the width of Δ. For the estimation of these values, the spin wave velocity is assumed to be, $c_{sw} = 1.6J$. The mass term is evaluated as $m \simeq 1.3J$ from the ARPES experiments by fitting the dispersion near $(\pi/2, \pi/2)$. The gauge charge is simply taken from the factor of the Maxwellian term obtained by integrating out the Dirac fermions: $e_a^2 = 3\pi m$. (If the same calculation is carried out for Dirac fermions with $k > k_0$, then the gauge charge value is $e_a^2 \simeq 3\pi^2 k_0/4$, for $k_0 \gg m$. Therefore, the above choice is the minimum value for the gauge coupling.) Recalling the fact that c_{sw} is taken unity in the above calculation, I found $E_s \simeq 2J$ and $\Delta \simeq 3J$. This value of Δ is consistent with the above assumption about k. The weight of the Gaussian spectrum is ~ 0.05 for this value of Δ. Because of the spin degrees of freedom and the degenerate nodes, the weight is ~ 0.2 in total. From the value of E_s, one can get insight about the strength of the coupling. If the system is in the (weak) strong coupling, the value of E_s is expected to be large (small). The fact that E_s is on the order of the band width suggests that the coupling is in the strong coupling regime.

IV. DISCUSSION

In this paper, the spectral function of the quasiparticle in the staggered flux state with phase fluctuations was computed within the effective theory described by the QED$_3$. It was shown that the quasiparticle spectra become a broad Gaussian form with an energy shift due to the gauge field interaction. The estimated spectrum width is consistent with the experiments. The analysis suggests that the coupling to the gauge field is in the strong coupling regime.

Since the model is based on the continuum approximation, the result is applicable to the quasiparticle excitations near $(\pm\pi/2, \pm\pi/2)$. However, the result is extended to other $\mathbf{k}$ points by formulating the theory on the lattice. Such a model is useful to study the change of the width of the spectra away from $(\pm\pi/2, \pm\pi/2)$.

As for the vertex correction, random phase approximation is applied with respect to the interaction arising from the longitudinal component of the gauge field. Of course, this is not the full vertex correction. In the long-wave length limit, there are other intermediate processes. However, it is expected that dominant contribution is covered by the above vertex correction because the longitudinal component plays a major role in screening the gauge charge.

Finally, let me comment on vanishing quasiparticle spectra observed in the experiments[1,2] along the line from $(\pi/2, \pi/2)$ to (π, π) and that from $(\pi, 0)$ to (π, π). A similar behavior is also observed in the pseudogap phase,[16] that is, only a part of the Fermi surface is observed as an arc shape.[17] One might expect that damping effect coming from the coupling to the gauge field leads to the suppression of the quasiparticle peaks. However, it turns out that the inclusion of a slight hopping term in the staggered flux state leads to the vanishing of the spectrum in the second magnetic Brillouin zone. I will discuss this matter in a future publication.

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APPENDIX A: DERIVATION OF QED$_3$ ACTION

In this appendix, I derive the QED$_3$ action as the effective theory for the $S = 1/2$ two-dimensional Heisenberg antiferromagnet:

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j. \tag{A1}$$

A fermion representation is introduced for the spin 1/2: $\mathbf{S}_{j\mu} = f^\dagger_{j\alpha}\sigma_{\alpha\beta} f_{j\beta}/2$ ($\mu = x, y, z$). σ^μ are the Pauli spin matrices. These fermions need to satisfy the constraint, $\sum_\alpha f^\dagger_{j\alpha} f_{j\alpha} = 1$. Introducing Lagrange multipliers to take into accout the constraint, the Hamiltonian is,

$$H = -\frac{1}{2} J \sum_{\langle i,j \rangle} f^\dagger_{i\alpha} f_{j\alpha} f^\dagger_{j\beta} f_{i\beta} + \sum_j \lambda_j \left(f^\dagger_{j\sigma} f_{j\sigma} - 2S \right), \tag{A2}$$

up to a constant term. The mean field taken in the π-flux state is $\chi_{ij} = \left\langle f^\dagger_{j\alpha} f_{i\alpha} \right\rangle$.h, by choosing a suitable gauge.[18] Since the system is homogeneous, uniform χ_{ij} and λ_j are assumed: $\chi_1 = \chi_{j+\hat{x},j}$, $\chi_2 = \chi_{j,j-\hat{y}}$, $\chi_3 = \chi_{j-\hat{x},j}$, and $\chi_4 = \chi_{j,j+\hat{y}}$, with j residing at an even site. Numerically solving the mean field equations for χ_j ($j = 1, 2, 3, 4$), with setting $\lambda = 0$, the π-flux state[10] is found in which $\chi_1\chi_2\chi_3\chi_4/|\chi_1\chi_2\chi_3\chi_4| = -1$.

The quasiparticle energy dispersion in the staggered flux state is

$$E_k = \pm\frac{J}{2} |\chi_1 \mathrm{e}^{-ik_x} + \chi_2^* \mathrm{e}^{ik_y} + \chi_3 \mathrm{e}^{ik_x} + \chi_4^* \mathrm{e}^{-ik_x}|. \tag{A3}$$

$|E_k|$ has minima at $(\pm\pi/2, \pm\pi/2)$, and around these points the energy dispersion has the relativistic form. Introducing the even and odd site fields, $f_{ek\alpha} = (f_{k\alpha} + f_{k+Q,\alpha})/\sqrt{2}$ and $f_{ok\alpha} = (f_{k\alpha} - f_{k+Q,\alpha})/\sqrt{2}$ with $Q = (\pi, \pi)$, and expanding E_k around $(\pm\pi/2, \pi/2)$, the Hamiltonian is rewritten as,

$$\begin{aligned} H \simeq\ & J {\sum_k}' \begin{pmatrix} f^\dagger_{e1k\alpha} & f^\dagger_{o1k\alpha} \end{pmatrix} \begin{pmatrix} 0 & -\chi_1^* k_x + \chi_2 k_y \\ -\chi_1 k_x + \chi_2^* k_y & 0 \end{pmatrix} \begin{pmatrix} f_{e1k\alpha} \\ f_{o1k\alpha} \end{pmatrix} \\ & + J {\sum_k}' \begin{pmatrix} f^\dagger_{e2k\alpha} & f^\dagger_{o2k\alpha} \end{pmatrix} \begin{pmatrix} 0 & \chi_1^* k_x + \chi_2 k_y \\ \chi_1 k_x + \chi_2^* k_y & 0 \end{pmatrix} \begin{pmatrix} f_{e2k\alpha} \\ f_{o2k\alpha} \end{pmatrix}. \end{aligned} \tag{A4}$$

Here the indices 1 and 2 are introduced to denote the fields around $(\pi/2, \pi/2)$ and those around $(-\pi/2, \pi/2)$. The summation with respect to k is taken over the magnetic Brillouin zone: $|k_x \pm k_y| < \pi$. Choosing $\chi_1 = \chi_3 = i|\chi|$ and $\chi_2 = \chi_4 = |\chi|$, and setting $\psi^\dagger_{k\alpha} = \left(f^\dagger_{e1k\alpha}, f^\dagger_{o1k\alpha}, f^\dagger_{o2k\alpha}, f^\dagger_{e2k\alpha} \right)$, the action is, in the continuum limit,

$$S = \int d^3x \overline{\psi}(x)\, i\gamma^\mu \partial_\mu \psi(x)\,, \tag{A5}$$

where $\overline{\psi} = \psi^\dagger \gamma^0$ and the γ matrices are

$$\gamma^0 = \begin{pmatrix} \tau_3 & 0 \\ 0 & -\tau_3 \end{pmatrix}, \quad \gamma^1 = \begin{pmatrix} i\tau_1 & 0 \\ 0 & -i\tau_1 \end{pmatrix}, \quad \gamma^2 = \begin{pmatrix} i\tau_2 & 0 \\ 0 & -i\tau_2 \end{pmatrix}.$$

Phase fluctuations about the staggered flux mean field state are included by the U(1) gauge field, a_μ, by replacing ∂_μ with $\partial_\mu - ia_\mu$. Integrating out the high-energy Dirac fermion fields with $k > k_0$ leads to the dynamics of the gauge field, which has the Maxwellian form. Numerically solving the Schwinger-Dyson equation, it is found that the self-energy has a non-zero mass.[13] Physically this mass is associated with the presence of the staggered magnetization which is absent at the mean field level. From the variational Monte Carlo approach with the finite mass m, it is shown that the mean field energy improves by the inclusion of m.[19,20] The action (2.1) is obtained by including the mass term arising from the staggered magnetization.

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